Massive and Massless Behavior in Dimerized Spin Ladders

D.C. Cabra[1,#] and M.D. Grynberg[2]
[1] *Physikalisches Institut der Universität Bonn, Nussallee 12, 53115 Bonn, Germany*
[2] *Departamento de Física, Universidad Nacional de la Plata, C.C. 67, (1900) La Plata, Argentina*

We investigate the conditions under which a gap vanishes in the spectrum of dimerized coupled spin-1/2 chains by means of Abelian bosonization and Lanczos diagonalization techniques. Although both interchain (J') and dimerization (δ) couplings favor a gapful phase, it is shown that a suitable choice of these interactions yields massless spin excitations. We also discuss the influence of different arrays of relative dimerization on the appearance of non-trivial magnetization plateaus.

PACS numbers: 75.10.Jm, 75.60.Ej Published in Phys. Rev. Lett. **82**, 1768 (1999).

Current developments in the field of spin ladders have revealed intriguing features of low-dimensional quantum antiferromagnets (AF) [1]. The appearance of plateaus in the magnetization curves of these systems has received much attention from both the theoretical and experimental side [2]. A necessary quantization condition for the appearance of such plateaus in generic ladders was derived in [2] (see also [3] for the case of 1D chains and [4–7] for other particular cases). In a very recent paper [8], an unexpected phenomenon has been observed in the magnetization curves of NH_4CuCl_3 at high magnetic fields. The crystal structure of this material at room temperatures is known to be composed of double chains (2-leg ladders), with three different nearest neighbor interactions. Thus, from previous theoretical studies of such arrange of couplings in ladders systems, plateaus at $\langle M\rangle = 0$ and 1/2 are expected to be visible at sufficiently low temperature. However, measurements performed in [8] at very low temperatures, clearly show two net plateaus at 1/4 and 3/4, while *no* plateaus are observed at the theoretically expected values $\langle M\rangle = 0$ and 1/2.

As a first step to reconcile some of these facts with the current understanding of ladder materials, in this work we study two important issues namely, (i) the possibility of closing the gap in a two-leg dimerized ladder by a combined effect of the dimerization and the interchain coupling and, (ii) the emergence of a plateau at $\langle M\rangle = 1/2$ depending on the realization of the relative dimerization (see Figs. 1(a)-(b)). Though (i) was studied on a qualitative level using non-linear sigma model techniques [9], here we present a quantitative and more systematic treatment, whereas (ii) is analyzed for the first time in this work. These two issues could shed light in the study of the experimental measurements such as those performed in [8] as well as in related aspects of CuGeO chain compounds [10], in which dimerization becomes staggered between weakly coupled chains.

As is well known, the isotropic spin-1/2 Heisenberg chain is already in a critical state. Thus any relevant perturbation, such as the Peierls dimerization instability [11] or a weak interchain coupling [12], [13], can drastically alter the nature of the ground state, whereas a massive spin gap excitation appears simultaneously in the energy spectrum. Interestingly, it was suggested that a combined effect could lead to a massless regime [9].

In the present work we study this issue quantitatively by means of both bosonization and numerical techniques, and find that there exists indeed a fine-tuning of the couplings responsible for the appearance of massless lines. Though this is a fine-tuning effect, our result implies that there is a *finite* region of the coupling parameter space where the gap is expected to be small. Thus, when the latter becomes comparable with thermal fluctuations, measurement attempts of zero magnetization plateaus could be smeared out even at low temperatures.

In analyzing the abelian bosonization of spin-1/2 Heisenberg ladders, we follow a similar methodology developed as in [2,5], [13], [14], [15], which is particularly suitable to elucidate the behavior of weak coupling regimes. Specifically, here we study two dimerized spin chains interacting through a Hamiltonian

$$H = \sum_{a,n} J_n^{(a)}\ \vec{S}_n^{\,(a)} \cdot \vec{S}_{n+1}^{\,(a)} + J' \sum_n \vec{S}_n^{(1)} \cdot \vec{S}_n^{(2)}\,, \quad (1)$$

($a = 1, 2$), where the $\vec{S}_n$ denote spin-1/2 operators. For *staggered* ladders, e.g. Fig. 1(a), the array of coupling exchanges are set as $J_n^{(2)} \equiv J_{n+1}^{(1)}$, and parametrized by $J_n^{(1)} = J\,[\,1 + (-1)^n\delta\,]$ say for chain (1), whereas for the non-staggered situation we just set $J_n^{(2)} \equiv J_n^{(1)}$, as shown in Fig. 1(b). To maintain pure AF and non-frustrated exchanges, the dimerization parameter is kept bounded by $|\delta| < 1$ throughout the $2L$ spins of the ladder length with periodic boundary conditions (L even).

On general grounds [2], it is expected that gapful magnetic excitations should appear for all magnetizations $\langle M\rangle \equiv \frac{1}{L}\sum_n \langle S_n^{z\,(1)} + S_n^{z\,(2)}\rangle$, satisfying the quantization condition $pN(1 - \langle M\rangle)/2 \in \mathcal{Z}$, where p stands for the polymerization [6] and N for the number of chains coupled together. This would imply the existence of plateaus at $\langle M\rangle = 0$ and, if dimerization occurs ($p = 2$), also at $\langle M\rangle = 1/2$, for a $N = 2$-leg ladder material such as the one studied in [8]. However, the experimental magnetization curve shows no plateaus at these two values of the magnetization, but instead at $\langle M\rangle = 1/4$ and $\langle M\rangle = 3/4$ [8]. To explain this apparent breakdown, we are especially interested to include an homogeneous field term of the type $-\frac{h}{2}\sum_n \left[S_n^{z\,(1)} + S_n^{z\,(2)}\right]$, so as to unravel the

interplay between the above kinds of coupling arrays and applied magnetic fields h, say along the z-direction.

It is well known that the low-energy properties of the Heisenberg chain, ($\delta = 0$), are described by a $c = 1$ conformal field theory of a free bosonic field compactified at radius $R = R(\langle M \rangle, \Delta)$ [2,4,5,14,15], for any given magnetization $\langle M \rangle$ and XXZ anisotropy $|\Delta| < 1$ (see e.g. [16]). The functional dependence of R can be obtained using the exact Bethe Ansatz solution by solving a set of integral equations obtained in [17,18] and [19] (for a fuller review consult for instance Ref. [2]). The bosonized expression of the low-energy effective Hamiltonian for a single homogeneous chain, ($\delta = 0$), in the presence of an external magnetic field h and with an XXZ anisotropy $-1 < \Delta < 1$, can be shown to adopt the form

$$\bar{H} = \int \mathrm{d}x \frac{\pi}{2} \left\{ \Pi^2(x)/(4R)^2 + R^2 \left(\partial_x \phi(x) \right)^2 \right\} , \quad (2)$$

with $\Pi = \partial_x \tilde{\phi}$, and $\phi = \phi_L + \phi_R$, $\tilde{\phi} = \phi_L - \phi_R$. Here, the effect of the magnetic field h and the XXZ anisotropy Δ enter through the radius of compactification R. This radius governs the conformal dimensions, in particular the conformal dimension of a vertex operator $\mathrm{e}^{i\beta\phi}$ is given by $\left(\frac{\beta}{4\pi R} \right)^2$.

In the limit of both weak dimerization $|\delta| \ll 1$, and interchain coupling $J'/J \ll 1$, the bosonized action reads

$$\begin{aligned} H_{int} \approx \lambda_1 \sum_x \partial_x \phi^{(1)} \partial_x \phi^{(2)} + \\ \lambda_2 \sum_x \cos(4k_F x + \sqrt{4\pi}(\phi^{(1)} + \phi^{(2)})) + \\ \lambda_3 \sum_x \cos(\sqrt{4\pi}(\phi^{(1)} - \phi^{(2)})) + \\ \lambda_4 \sum_x \cos(\sqrt{\pi}(\tilde{\phi}^{(1)} - \tilde{\phi}^{(2)})) + \\ \sum_{(a)=1}^{2} \sum_x \alpha^{(a)} (-1)^x \cos(2k_F(x+1/2) + \sqrt{4\pi}\, \phi^{(a)}(x)) \,. \end{aligned} \quad (3)$$

where $\lambda_i \propto J'/J$, $\alpha^{(1)} \propto \delta$ and $\alpha^{(2)} \propto \pm\delta$, (the minus sign corresponding to Fig. 1a), and the Fermi momentum k_F is related to the total magnetization $\langle M \rangle$ via $k_F = (1 - \langle M \rangle)\pi/2$. In (3) a marginal term has been neglected for the sake of simplicity since it does not change our results.

(i) Closing of the gap

At zero magnetization (i.e. $k_F = \pi/2$), all terms in (3) are commensurate and relevant. Due to the λ_1 term, we have to first diagonalize the derivative part of the Hamiltonian which is achieved by introducing new variables $\phi^{\pm} = (\phi^1 \pm \phi^2)/\sqrt{2}$. The associated compactification radii are given by $R_{\pm} = R\sqrt{1 \pm J'/(4J\pi^2 R^2)}$.

For AF interchain coupling, ($J' > 0$), and in the new basis, the λ_4 term is the most relevant and orders the $\tilde{\phi}^-$ field (the dimerization terms mix the ϕ^+ and ϕ^- variables and will be treated as a perturbation). The α interaction in (3) is then wiped out after integrating the massive ϕ^- field, since it always contains a contribution from ϕ^-. Thus we are left with the ϕ^+ field with a relevant interaction given by λ_2. Hence, this field is in general massive so we can expect a plateau at zero magnetization. The interesting point here is that the α interaction generates radiatively a term that can cancel the λ_2 perturbation, (which is the one responsible for the mass of the symmetric boson). From this plain weak coupling analysis we see that this happens on the critical line given by

$$\frac{J'}{J} \propto \delta^2 \,. \quad (4)$$

Therefore, whenever this cancellation occurs we have one massless degree of freedom corresponding to the symmetric combination of the original free bosons ϕ^+.

To enable an independent check of this result, we now turn to a numerical finite-size analysis of the original ladder Hamiltonian. We direct the reader's attention to Fig. 2 where we display the energy gap necessary to create an excitation with total spin $S = 1$ in the staggered coupling array [Fig. 1(a)]. The results were obtained from exact diagonalizations of finite ladder lengths, $4 \le L \le 12$, via a recursion type Lanczos algorithm [20]. In studying the mass gap extrapolations towards their thermodynamic limits (dashed curve of Fig. 2), we fitted the whole set of finite-size results using a variety of standard procedures; namely linear, logarithmic and van den Broeck-Schwartz type methodologies of convergence [21]. Basically, they yield analogous results with at least 2 significant digits, though within the neighborhood of the massless region finite size effects become noticeable. In particular, this latter variation is reflected in the localization of the critical line contained within the error bars of Fig. 3. Nevertheless, at least in the weak coupling (δ, J') regime we were able to obtain a reasonable agreement with Eq. (4). The progressive departure from the latter however, yields the right critical parameters. As $|\delta| \to 1$, we clearly recover the "snake chain" limit where criticality is achieved when $J' = 2J$ [see Fig. 1(a)]. This strong coupling regime yields in turn the expected linear behavior in $(|\delta| - 1)$.

Preliminary estimations of the sound velocity [22] near the ground state are consistent with a conformal anomaly $c = 1$ throughout the critical line, except for $\delta = J' = 0$, where the system has two decoupled bosons with $c = 2$. Moreover, a low temperature computation of the magnetic susceptibility revealed that the latter is enhanced significantly on approaching the massless line (4), thus lending further support to our bosonization approach.

Also, this effect is presumed to occur on the ferromagnetic side, $J' < 0$, where a critical line can emerge with usual dimerization as well [Fig. 1(b)]. In fact, a similar analysis using the perturbative RG approach has been given in the first reference of [13] and, indeed, the effect is observed numerically [23].

(ii) Plateau at $\langle M \rangle = 1/2$

Let us now consider Eq. (3) at non-zero magnetization $\langle M \rangle$. As was referred to above, this can be readily accounted through the radius of compactification $R(\langle M \rangle, \Delta)$ resulting from the effect of the magnetic field h and the Fermi momentum $k_F = (1 - \langle M \rangle)\pi/2$. Then, the λ_2 and α interactions are incommensurate, and we have in principle a massless mode corresponding to the ϕ^+ field. However an interesting phenomenon can be observed: a plateau in the magnetization curve is expected to appear at 1/2 of the saturation value due to the appearance of the radiative correction

$$\gamma \sum_{x=1}^{L} (-1)^x \cos(4k_F(x + 1/2) + \sqrt{8\pi}\phi^+). \tag{5}$$

This term is generated from a combined effect of the dimerization on each chain ($\alpha^{(a)}$ interactions in (3)) and the interchain interaction terms $\langle M \rangle \left(\cos(2k_F x + \sqrt{4\pi}\phi^{(1)}) + \cos(2k_F x + \sqrt{4\pi}\phi^{(2)})\right)$.

However, the presence of this radiatively generated term is strongly dependent of the *manner* in which the dimerization is realized. In the case of normal dimerization, one finds that $\gamma \propto \delta J' \langle M \rangle$, while in the staggered case it vanishes exactly, $\gamma \equiv 0$, due to the relative minus sign between $\alpha^{(1)}$ and $\alpha^{(2)}$. This effect, predicted from our weak coupling analysis can be clearly observed by comparing Figs. 4(a) and 4(b) (see below).

The operator (5) is relevant for any anisotropy $\Delta > 0$, where a Kosterlitz-Thouless (KT) transition is expected to take place. (More precisely, this KT point will depend also on the interchain coupling J' through $R_\pm$

One can also understand this difference in a sort of strong coupling limit, when $|\delta| \to 1$. It can be readily checked that the normal dimerization displays an $\langle M \rangle = 1/2$ plateau $\forall h \in (2J, 4J)$ with $J' = J$, while there is no plateau in the staggered array. This effect is therefore robust in the sense that it is valid for all values of the couplings and could then be a useful tool for experimentalists [8] to decide whether the former or the latter exchange topology is actually realized in a given compound.

To test the correctness of this scenario, finally we recur to the Lanczos algorithm, to obtain the lowest energy eigenvalues on each magnetization subspace $S^z = \{0, 1, \ldots, L\}$. Using ladders up to $L = 12$, in Figs. 4(a) and (b) we display respectively the ground state magnetization curves of the staggered and normal coupling arrays. By setting $J'/J = 2$ and $\delta = 0.5$, our numerical analysis supports entirely the bosonization picture as *no* plateau shows up for staggered arrays at any finite magnetization [Fig. 4(a)]. In contrast, the normal array [Fig. 4(b)] clearly exhibits the expected $\langle M \rangle = 1/2$ plateau. Furthermore, the *robustness* of this result was checked numerically for a variety of dimerization (δ) and interchain (J') coupling regimes. In all cases, the staggered (normal) array always displays a massless (massive) behavior at $\langle M \rangle = 1/2$. Finally, it is worth remarking that this study of the simplest $N = 2$ leg ladder and with dimerization, ($p = 2$ in the notation of [6]), can be extended using the same bosonization methods to the study of N leg ladders with arbitrary polymerization p [23].

In summary, by using bosonization and numerical techniques, we have studied two interesting phenomena occurring in a dimerized two-leg ladder: (i) the closing of the gap at zero magnetization by means of a fine-tuning mechanism and, (ii) the disappearance of the 1/2 plateau (gap at finite $\langle M \rangle$) by alternating the dimerization of the chains along the rung direction. As for the first issue, we presented a thorough quantitative study of this phenomenon for AF systems, whereas (ii) was studied for the first time here. On this latter respect, though NH_4CuCl_3 under high magnetic fields is supposed to be described by a two-leg ladder system, its magnetization curves does not show up neither $\langle M \rangle = 0$ nor $\langle M \rangle = 1/2$ plateaus [8]. We trust the present paper will help to convey a better understanding of these ladder materials.

It is a pleasure to acknowledge fruitful discussions with A. Dobry, A. Honecker, A.A Nersesyan, P. Pujol and V. Rittenberg. The authors acknowledge partial financial support of CONICET, Fundación Antorchas and Deutsche Ausgleichbank. D.C.C. would like to thank the DAAD for financial support under the Visiting Professors Programme and the Physikalisches Institut der Universität Bonn for hospitality. This work is done under ANPCyT project No. 03-00000-02249.

On leave of absence from the Universidad Nacional de La Plata and Universidad Nacional de Lomas de Zamora, Argentina.

[1] The status of the field has been reviewed by T.M. Rice, Z. Phys. **B 103**, 165 (1997); E. Dagotto, T.M. Rice, Science **271**, 618 (1996).
[2] D.C. Cabra, A. Honecker, P. Pujol, Phys. Rev. Lett. **79**, 5126 (1997); Phys. Rev. **B58**, 6241 (1998) and references therein.
[3] M. Oshikawa, M. Yamanaka, I. Affleck, Phys. Rev. Lett. **78**, 1984 (1997).
[4] K. Totsuka, Phys. Lett. **A228**, 103 (1997).
[5] K. Totsuka, Phys. Rev. **B57**, 3454 (1998).
[6] D.C. Cabra, M.D. Grynberg, Phys. Rev. **B59**, 119 (1999).
[7] A. Honecker, Phys. Rev. **B** in press (1999).
[8] W. Shiramura *et al.*, J. Phys. Soc. Jpn. **67**, 1548 (1998).
[9] M.A. Martín-Delgado, R. Shankar, G. Sierra, Phys. Rev. Lett. **77**, 3443 (1996).
[10] J. P. Boucher, L.P. Regnault, J. Phys. I (Paris) **6**, 1939 (1996).
[11] M.C. Cross, D.S. Fisher, Phys. Rev. **B19**, 402 (1979). See also J. Riera, A. Dobry Phys. Rev. **B51**, 16098 (1995); G. Castilla, S. Chakravorty, V.J. Emery, Phys. Rev. Lett. **75**, 1823 (1995).

[12] E. Dagotto, J. Riera, D.J. Scalapino, Phys. Rev. **B47**, 5744 (1992).
[13] K. Totsuka, M. Suzuki, J. Phys. Cond. Matt. **7**, 6079 (1995); D.G. Shelton, A.A. Nersesyan, A.M. Tsvelik, Phys. Rev. **B53**, 8521 (1996).
[14] I. Affleck, in *Fields, Strings and Critical Phenomena, Les Houches, Session XLIX*, edited by E. Brezin and J. Zinn-Justin (North-Holland, Amsterdam, 1988).
[15] H.J. Schulz, Phys. Rev. **B34**, 6372 (1986).
[16] F.D.M. Haldane, Phys. Rev. Lett. **45**, 1358 (1980).
[17] F. Woynarovich, H.-P. Eckle, T.T. Truong, J. Phys. A: Math. Gen. **22**, 4027 (1989).
[18] N.M. Bogoliubov, A.G. Izergin, V.E. Korepin, Nucl. Phys. **B275**, 687 (1986).
[19] V.E. Korepin, N.M. Bogoliubov, A.G. Izergin, *Quantum Inverse Scattering Method and Correlation Functions*, Cambridge University Press, Cambridge (1993).
[20] G.H. Golub, C.F. Van Loan, *"Matrix Computations"*, 3rd ed. (Johns Hopkins University Press, Baltimore 1996).
[21] A.J. Guttmann in *Phase Transitions and Critical Phenomena*, edited by C. Domb, J. Lebowitz (Academic Press, New York 1990), Vol. 13. Consult also C.J. Hamer, M.N. Barber, J. Phys. **A14**, 2009 (1981).
[22] J. L. Cardy, J. Phys. **A 17**, L385 (1984); H. W. Blöte, J. L. Cardy, M. P. Nightingale, Phys. Rev. Lett. **56**, 742 (1986) ; I. Affleck, Phys. Rev. Lett. **56**, 746 (1986).
[23] D.C. Cabra, M.D. Grynberg, in preparation.

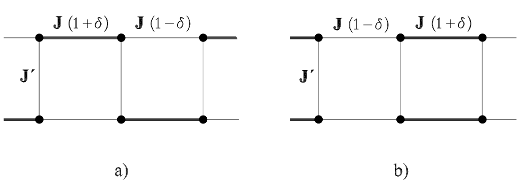


FIG. 1. Schematic view of alternating ladders with inter-chain coupling J' and dimerization parameter δ for (a) staggered and, (b) non-staggered arrays

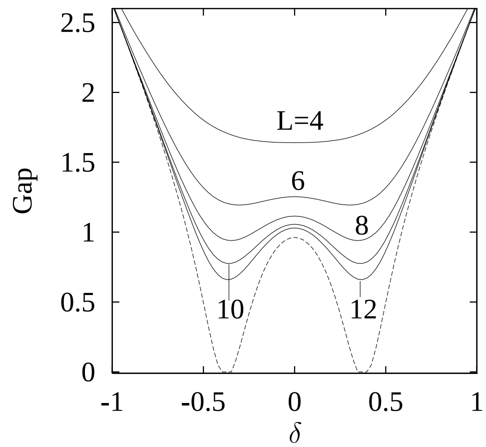


FIG. 2. Gap spectrum for different sizes of the staggered spin ladder for $J'/J = 1$. The dashed lines display extrapolations to the thermodynamic limit.

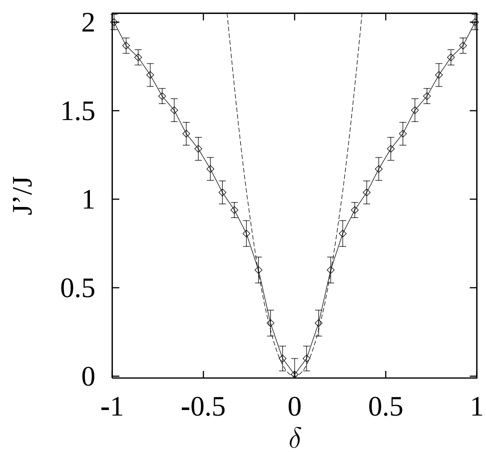
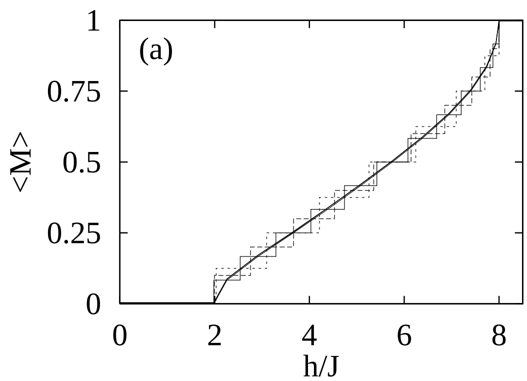


FIG. 3. Critical line of the staggered spin ladder in the (δ, J') coupling parameter space, extrapolated from finite samples. Solid lines are guide to the eye whereas the dashed parabola stands for the bosonization approach.



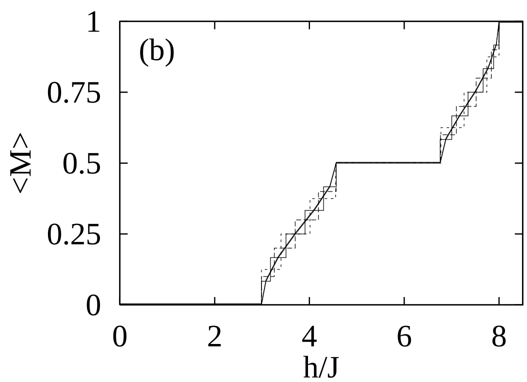


FIG. 4. Magnetization curves of dimerized ladders for $\delta = 0.5$ and $J'/J = 2$ using both (a) staggered and, (b) non-staggered coupling arrays. Solid, dashed and short dashed lines denote respectively magnetizations for $L = 12$,10 and 8. The thick full line denotes the expected form in the thermodynamic limit